

## FINAL REPORT

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## THE STRUCTURE OF PARTICLE CLOUD PREMIXED FLAMES

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## ABSTRACT

The structure of premixed flames propagating in combustible systems, containing uniformly distributed volatile fuel particles, in an oxidizing gas mixture is analyzed. This analysis is motivated by experiments conducted at NASA Lewis Research Center on the structure of flames propagating in combustible mixtures of lycopodium particles and air. Several interesting modes of flame propagation were observed in these experiments depending on the number density and the initial size of the fuel particle. The experimental results show that steady flame propagation occurs even if the initial equivalence ratio of the combustible mixture based on the gaseous fuel available in the particles,  $\phi_u$  is substantially larger than unity. A model is developed to explain these experimental observations. In the model it is presumed that the fuel particles vaporize first to yield a gaseous fuel of known chemical composition which then reacts with oxygen in a one-step overall process. The activation energy of the chemical reaction is presumed to be large. The activation energy characterizing the kinetics of vaporization is also presumed to be large. The equations governing the structure of the flame were integrated numerically. It is shown that the interplay of vaporization kinetics and oxidation process, can result in steady flame propagation in combustible mixtures where the value of  $\phi_u$  is substantially larger than unity. This prediction is in agreement with experimental observations.

1. Introduction.

The aim of this study is to provide a numerical and asymptotic description of the structure of planar laminar flames, propagating in a

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medium containing a uniform cloud of fuel-particles premixed with air. Attention is restricted here to systems where the fuel-particles first vaporize to form a known gaseous fuel, which is then oxidized in the gas-phase. This research was supported for the period September 14, 1991 to September 13, 1992. This research was performed in collaboration with Professor A. Linan at Instituto Nacional de Tecnica Aeroespacial and Escuela Tecnica Superior de Ingenieros Aeronauticos, Madrid Spain.

The model developed here is built on previous asymptotic analysis structure of premixed particle-cloud flames [1]. In this previous analysis the vaporization rate of the fuel-particles was presumed to be proportional to  $T_s^{1.33}$ , where  $T_s$  is the temperature of the fuel-particles. Hence, the activation temperature in an Arrhenius-type rate law for the vaporization process is not large. For simplicity, the temperature of the fuel-particles was presumed to be equal to the gas temperature. The analysis was performed for values of  $\phi_u > 1.0$ , where  $\phi_u$  is the equivalence ratio based on the gaseous fuel available in the particles. For given values of  $\phi_u$  the analysis yields results for the burning velocity and  $\phi_g$ , where  $\phi_g$  is the effective equivalence ratio in the reaction zone [1]. The analysis shows that even though  $\phi_u > 1.0$ , for certain cases the calculated value of  $\phi_g$  is less than unity.

A two-temperature model is described here, where the temperature of the fuel-particles is different from the temperature of the gas. However the size of the fuel-particle is assumed to be small enough so that its velocity is nearly equal to the gas velocity. A general treatment of flame propagation supported by volatile fuel-particles should consider both radiative and molecular transport mechanisms, the temperature difference and the differences in velocity between the gas and the particulates, the nonadiabaticity of combustible systems of finite size, as well as the detailed kinetics of oxidation and the kinetics of vaporization pyrolysis. This work has the somewhat limited aim of examining the interplay of vaporization kinetic and oxidative kinetic processes for cases where nonadiabatic and radiative transport mechanisms are not substantial.

## 2. Formulation.

A model is developed to describe steady, one-dimensional, planar flame propagation in a combustible mixture consisting of uniformly distributed fuel-particles in air. The initial number density of the particles,  $n_u$  (number of particles per unit volume) and the initial radius  $a_u$  are presumed to be known. All external forces including gravitational forces effects are assumed to be negligible. The kinetics of vaporization of a fuel-particle is represented by the expression

$$\dot{m} = 4 \pi a^2 A \exp\left(-\frac{T_{av}}{T_s}\right) = -\frac{4}{3} \pi \frac{d(a^3)}{dt} \rho_s, \quad (1)$$

where  $\dot{m}$  represents the mass of gaseous fuel vaporized per unit time from the fuel-particle,  $a$  and  $\rho_s$  are the instantaneous radius and density respectively of a fuel-particle. The rate parameters  $A$  and  $T_{av}$  which respectively represent the frequency factor and the activation temperature of the vaporization process are presumed to be known. The ratio  $T_{av}/T_s$  is presumed to be a large quantity.

Consider a vaporizing fuel-particle in an ambient atmosphere. The balance equation for the mass fraction of the gaseous fuel vaporizing from the fuel-particle  $Y_F$ , and the energy balance equation can be written as,

$$\frac{\dot{m}}{4 \pi r^2} \frac{\partial Y_F}{\partial r} - \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{k}{c_p L_F} \frac{\partial Y_F}{\partial r} \right) = 0, \quad (2)$$

$$\frac{\dot{m}}{4 \pi r^2} \frac{\partial (c_p T)}{\partial r} - \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 k \frac{\partial T}{\partial r} \right) = 0, \quad (3)$$

where  $r$  is the radial coordinate. For the gas mixture  $k$  is the thermal conductivity,  $c_p$  the heat capacity, and  $T$  the temperature. The quantity  $L_F = k/(\rho c_p D_F)$  is the Lewis number of the gaseous fuel which is presumed to be a constant and  $D_F$  is the diffusion coefficient of the gaseous fuel. Boundary conditions for Eqs. 2 and 3 far from the surface of the fuel-particle, and at the surface of the fuel-particle can be written as,

$$\begin{aligned} T &= T_\infty, Y_F = Y_{F,\infty} \text{ as } r \rightarrow \infty, \\ T &= T_s, \dot{m}(1 - Y_F) = -\frac{4\pi k r^2}{c_p L_F} \frac{\partial Y_F}{\partial r} \text{ at } r = a. \end{aligned} \quad (4)$$

The values of  $T_\infty$  and  $Y_{F,\infty}$  will be determined from the solution of the equations governing the structure of the laminar flame. The temperature of the fuel-particle  $T_s$  can be calculated from the energy balance equation

$$q_g = \left( 4\pi r^2 k \frac{\partial T}{\partial r} \right)_{r=a} = \dot{m} L_v + \frac{4}{3} \pi a^3 \rho_s c_s \frac{dT_s}{dt}, \quad (5)$$

where  $t$  represents the time,  $c_s$  represents the heat capacity of fuel-particle, and  $L_v$  represents the heat required to vaporize unit mass of vapor from a fuel-particle. The values of  $c_p$  and  $c_s$  are presumed to be constant. If the value of  $k$  is also presumed to be constant, then from integration of Eqs. 2 and 3, using Eq. 4 to determine the constants of integration, the profiles of  $Y_F$  and  $T$  can be expressed as

$$Y_F = 1 - (1 - Y_{F,\infty}) \exp\left(-\frac{\dot{m} c_p L_F}{4\pi k r}\right), \quad (6)$$

and

$$T = T_s - \frac{q_g}{c_p \dot{m}} + \left( T_\infty - T_s + \frac{q_g}{c_p \dot{m}} \right) \exp\left(-\frac{\dot{m} c_p}{4\pi k r}\right). \quad (7)$$

Introducing the definition,

$$\lambda = \left( \frac{\dot{m} c_p}{4\pi k r} \right)_{r=a}, \quad (8)$$

from Eqs. 5 and 7 it follows that

$$\frac{4\pi a k \lambda (T_\infty - T_s)}{\exp(\lambda) - 1} = \frac{4\pi a k L_v \lambda}{c_p} + \frac{4}{3} \pi a^3 \rho_s c_s \frac{dT_s}{dt}. \quad (9)$$

The term on the left side of Eq. 9 denotes the rate of heat transfer from the gas to the fuel-particle, with the effective Nusselt's number denoted by  $\lambda/[\exp(\lambda) - 1]$ . The first term following the equality sign on the right side of Eq. 9 denotes the latent heat required to vaporize the fuel-particle, and the second term denotes the sensible heat required to raise the temperature of the fuel-particle. It follows from Eqs. 1, and 8 that

$$\lambda = \frac{a c_p}{k} A \exp\left(-\frac{T_{av}}{T_s}\right). \quad (10)$$

Let  $T_v$  denote a characteristic value of the temperature of the fuel-particle for which the value of  $\lambda$  evaluated from Eq. 10 is of order unity. For  $T_s < T_v$ , the vaporization rate and consequently the value of  $\lambda$ , is exponentially small. In the limit of small values of  $\lambda$ ,  $\lambda/[\exp(\lambda) - 1] = 1$ . Hence the first term on the right side of Eq. 9 can be neglected in calculating the value of  $T_s$ . For  $T_s = T_v$ ,  $\lambda$  is of order unity. If the value of  $T_s$  is allowed to increase beyond  $T_v$ , then the value of  $\lambda$  would become exponentially large and the term on the left side of Eq. 9 would become exponentially small, consequently the rate of heat transfer from the gas-phase to the solid, will be small. Therefore, for values of  $T_s$  beyond  $T_v$ , the value of the derivative  $dT_s/dt$  will be negligibly small, so that the value of  $\lambda$  remains of order unity. For simplicity, it is presumed that  $\dot{m} = 0$  for  $T_s < T_v$  and the value of  $T_s$  does not increase after it attains the value  $T_v$ .

The governing equations for the structure of the flame can be written as,

$$V = \rho_u u_u + \frac{4}{3} \pi \rho_s n_u u_u (a_u^3 - a^3), \quad (11)$$

$$\frac{d(V Y_F)}{dx} - \frac{k_u}{c_p L_F} \frac{d^2 Y_F}{dx^2} = \frac{n_u \rho_u u_u}{V} \dot{m} - w_F \frac{\rho_u}{\rho}, \quad (12)$$

$$\frac{d(V Y_{O_2})}{dx} - \frac{k_u}{c_p L_{O_2}} \frac{d^2 Y_{O_2}}{dx^2} = -w_{O_2} \frac{\rho_u}{\rho}, \quad (13)$$

$$\frac{d(V c_p T)}{dx} - k_u \frac{d^2 T}{dx^2} = \frac{n_u \rho_u u_u}{V} q_p + Q_R w_F \frac{\rho_u}{\rho}. \quad (14)$$

Here the subscript u denotes conditions in the ambient reactant stream. The subscript  $\infty$  has been dropped from the quantities  $Y_F$ ,  $Y_{O_2}$  and  $T$  appearing in Eqs. 12-14. The quantities  $w_F$  and  $w_{O_2}$  denote the rate of consumption of gaseous fuel and oxygen per unit volume, and  $Q_R$  is the heat released per unit mass of gaseous fuel consumed. The independent variable  $x$  is related to the spatial coordinate  $x'$  as,

$$x = \int_0^x \left( \frac{\rho}{\rho_u} \right) dx'. \quad (15)$$

In the regions where  $T_s < T_v$ , the vaporization rates are assumed to be negligibly small hence the radius of the fuel-particle does not change and its temperature  $T_s$  and the quantity  $q_p$  can be calculated from the relations,

$$a_u^2 \frac{\rho_s c_s V}{\rho_u} \frac{dT_s}{dx} = \frac{3 k_u}{2 T_u} (T^2 - T_s^2), \quad (16)$$

and

$$q_p = -\frac{4}{3} \pi a_u^3 \rho_s c_s \frac{V}{\rho_u} \frac{dT_s}{dx}. \quad (17)$$

When the value of the temperature of the fuel-particle reaches  $T_v$ , they begin to vaporize and the increase in their temperature is negligibly small. The radius of the fuel-particle and the quantity  $q_p$  can be calculated from the expressions,

$$a \frac{da}{dx} = -\frac{k_u \rho_u}{T_u c_p \rho_s V} \left[ T - T_v + \left( T_v - \frac{L_v}{c_p} \right) \ln \left( 1 + \frac{c_p (T - T_v)}{L_v} \right) \right], \quad (18)$$

and,

$$q_p = \dot{m} (c_p T_v - L_v), \quad \dot{m} = -\rho_s \frac{4}{3} \pi \frac{V}{\rho_u} \frac{d(a^3)}{dx}. \quad (19)$$

In deducing the system of equations 12-19 the product  $\rho k$  was presumed to be a constant. The chemical reaction between the gaseous fuel and the oxidizer is presumed to occur by a one-step process. The system of equations 12-19 were solved numerically.

### 3. Results

For purpose of illustration calculations were performed assuming that the gaseous fuel that evolves from the fuel-particle is methane. The chemical kinetic rate parameters characterizing the gas-phase oxidation were chosen such that the burning velocity for stoichiometric mixture of gaseous methane and air is 37 cm/s. The values of some of the parameters used in the calculations are  $k_u = 0.00005 \text{ cal}/(\text{cm s K})$ ,  $\rho_u = 0.001135 \text{ g/cm}^3$ ,  $\rho_s = 1.0 \text{ g/cm}^3$ ,  $T_u = 298 \text{ K}$ ,  $T_v = 600 \text{ K}$ ,  $L_v/Q_R = 0.01$ . Results for the burning velocity  $u_u$  as a function of the equivalence ratio  $\phi_u$ , calculated based on the gaseous fuel available in the fuel-particles, for values of  $a_u$  equal to 1.0  $\mu\text{m}$ , 3.0  $\mu\text{m}$ , and 5.0  $\mu\text{m}$  are shown in Fig. 1. Figure 1 shows that steady flame propagation is possible in fuel-rich combustible mixtures and the value of  $u_u$  initially increases with increasing values of  $\phi_u$  attains a maximum value then begins to decrease. In Fig. 2 the structure of the flame is plotted at a value of  $\phi_u = 1.8$  and  $a_u = 3.0 \mu\text{m}$  and corresponds to the region where the value of  $u_u$  increases with increasing values of  $\phi_u$ . The various non-dimensional quantities appearing in this figure are defined as,

$$\begin{aligned} z &= \frac{\rho_u u_u c_p}{k_u} x, \quad \theta = \frac{T - T_u}{T_b - T_u}, \quad \theta_s = \frac{T_s - T_u}{T_b - T_u}, \\ \alpha &= \frac{a}{a_u}, \quad y_F = \frac{4 Y_F}{Y_{O_{2u}}}, \quad y_{O_2} = \frac{Y_{O_2}}{Y_{O_{2u}}}. \end{aligned} \quad (20)$$

where  $T_b$  is the adiabatic flame temperature. Figure 2 shows that gaseous fuel is the limiting reactant in this region. In Fig. 3 the structure of the flame is plotted at a value of  $\phi_u = 3.69$  and  $a_u = 3.0 \mu\text{m}$  and corresponds to the region where the value of  $u_u$  decreases with increasing values of  $\phi_u$ . Figure 3 shows that oxygen is the limiting reactant in this region.

### 4. Future Research.

Future research will be directed toward performing numerical calculations using the system of equations 12-18 over a wide parametric range. Asymptotic description of the flame structure will also be attempted.

## 5. References.

1). Seshadri, K., Berlad, A. L., and Tangirala, V., *The Structure of Particle-Cloud Flames*, Combustion and Flame **89**: 333-342 (1992)

## 6. List of Figures

Figure 1. The burning velocity  $u_u$  (cm/s) as a function of the equivalence ratio  $\phi_u$ , for various values for the initial radius of the fuel-particle  $a_u$ .

Figure 2. The structure of the flame for  $\phi_u = 1.8$  and  $a_u = 3.0 \mu\text{m}$ .

Figure 3. The structure of the flame for  $\phi_u = 3.69$  and  $a_u = 3.0 \mu\text{m}$ .



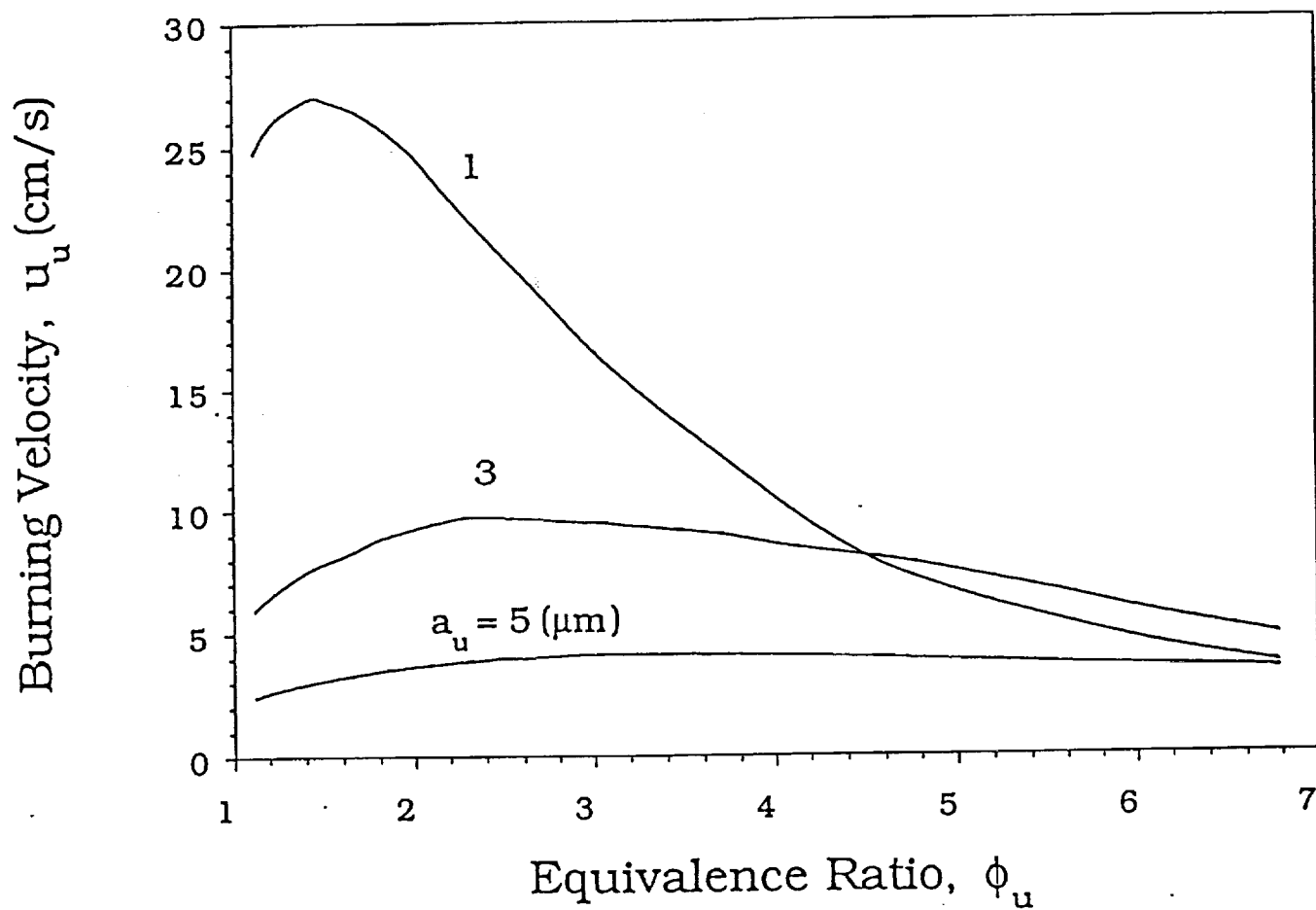


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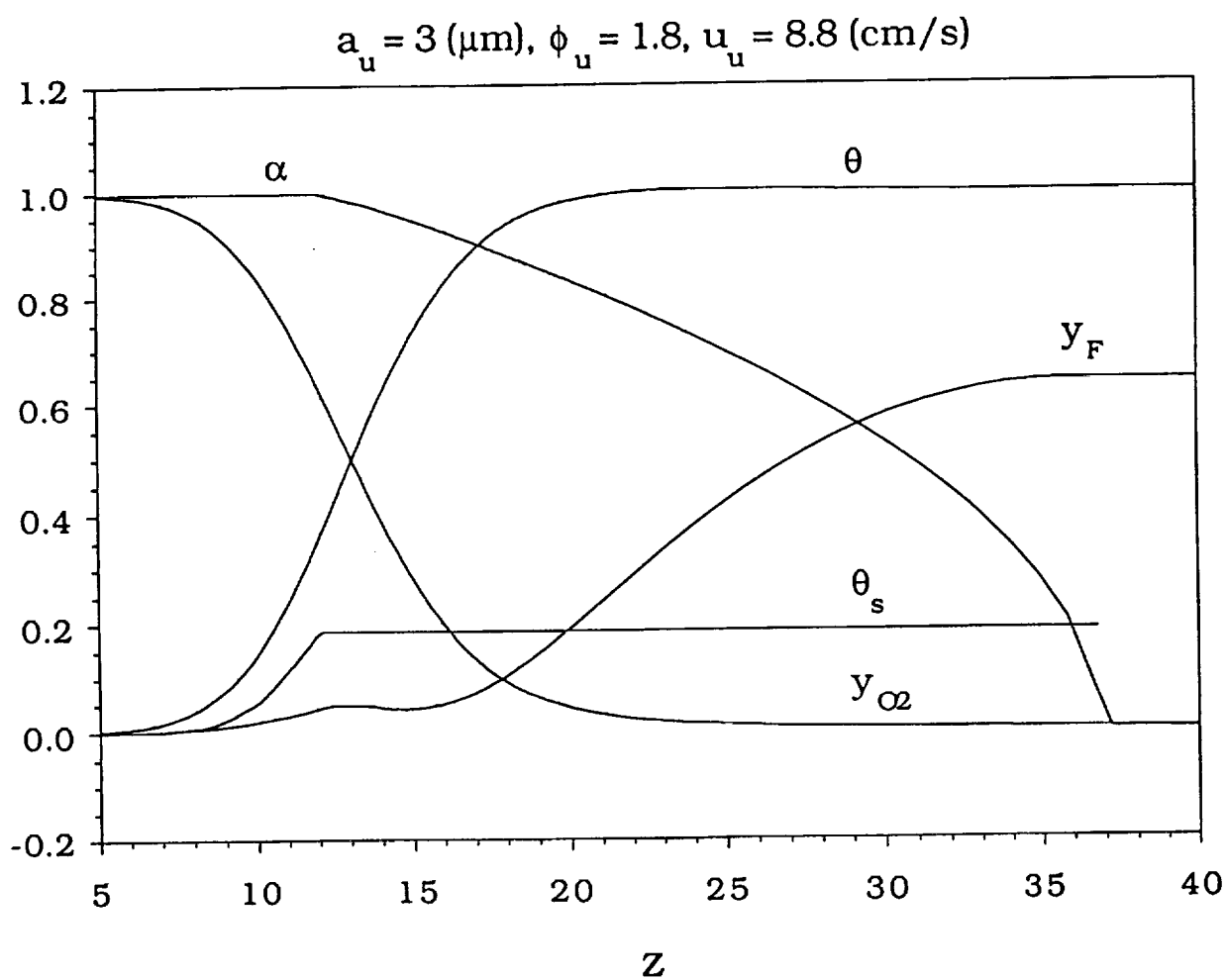


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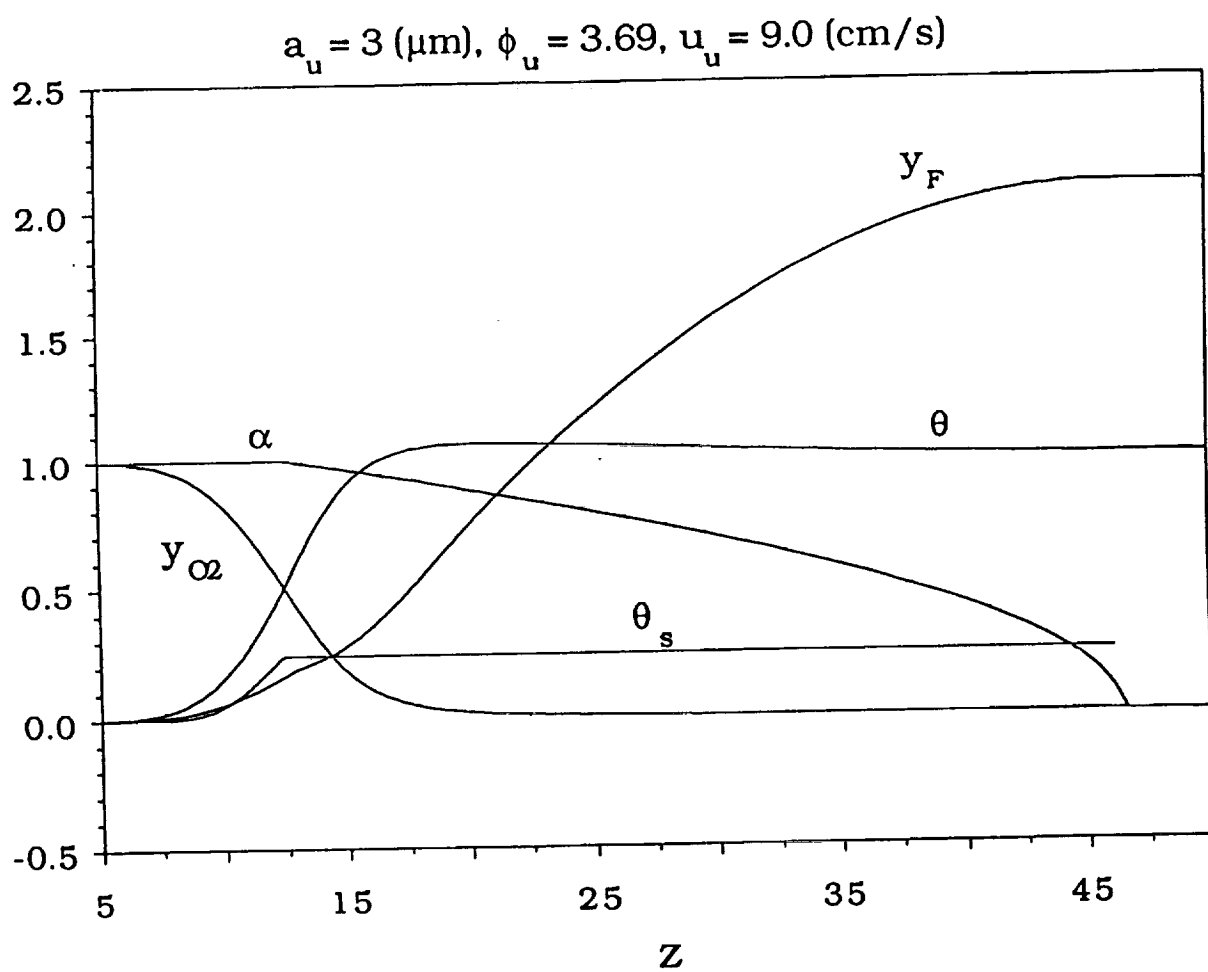


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